J. Fluid Mech. (1986), *vol.* 167, *pp.* 409–414
Printed in Great Britain

Combustion theory: a report on Euromech 203

By **J. F. CLARKE,** Colloquium Chairman,
Aerodynamics, Cranfield Institute of Technology, Bedford MK43 0AL

AND **N. RILEY**
School of Mathematics and Physics, University of East Anglia, Norwich NR4 7TJ

The 203rd Euromech Colloquium, on developments in the theoretical modelling of homogeneous and heterogeneous combustion was held at Cranfield Institute of Technology from 2 to 4 December 1985. The emphasis of the meeting was on the ability of analytic, numerical and approximate methods to predict, or interpret, events which occur in the laboratory or in the field. There were forty-five participants in the Colloquium from six different countries.

1. Introduction

In his opening remarks the Colloquium Chairman drew attention to the rapid advances that have been made over the past twenty years in our theoretical understanding of combustion phenomena and their associated fluid-mechanical processes. This was attributed, in large measure, to the exploitation of singular perturbation methods, in particular the methods of matched expansions and multiple scales. To emphasize this point attention was drawn to the two editions of Williams' book (1965, 1985). The first edition, which is based upon the substantial body of theoretical work that existed at that time, illustrated an absence of unity in the subject, the theoretical approach to which had been somewhat *ad hoc*. By contrast the second, and substantially revised, edition acknowledges the unifying part played by asymptotic methods in moving the subject forward.

There is, of course, a multiplicity of dimensionless parameters arising in combustion theory, especially since almost all burning takes place in the gas phase and one therefore needs to add information about chemistry to the usual set of parameters required to describe the associated fluid motions. The task of the mathematical modeller is both to seek out the parameter that is centrally significant to the physics of the problem under examination, and to relate all of the other parameters in the problem to it in sets of so-called distinguished limits. Properly handled, asymptotic methods display a unique resonance between mathematical method and the physics of the problem that not only illuminates the physics but also provides a basis for theoretical understanding beyond a first order of accuracy. As an example, the smallness of a Damköhler number, namely the ratio of a typical chemical time to a typical time for diffusion of reactants, has been successfully exploited to place the classical thin-sheet diffusion-flame model on to a firmer theoretical footing using the method of matched expansions. However, valuable though Damköhler-number asymptotics has proved to be, it throws no light on important topics such as ignition and extinction. Only when the smallness of the Damköhler number is related to the appearance of the exponential Arrhenius activation-energy factor are these wider considerations properly understood.

To be sure, asymptotic methods, central though they may be in current theoretical developments, are not all-embracing, as the contributions to the Colloquium demonstrate. These may be divided into five groups, namely classical ignition or explosion theory, two-phase flow problems, 'two-fluid' models related to questions raised by turbulent motions, gas dynamics and combustion, and the chemical kinetics of flame behaviour. This subdivision is adhered to in the sections below.

2. Thermal-explosion theory

The classical theory of thermal explosions, due to Frank–Kamenetskii, is a steady-state theory. With the assumption of zero-order chemical reaction the steady-state reaction-diffusion equations will only admit solutions for a range of values of the so-called Frank–Kamenetskii parameter (FKP). Beyond some critical value of FKP, when no steady states are available, thermal ignition is inevitable. In the opening lecture of the Colloquium, Adler addressed himself to three problems based upon the classical theory, all of which involved a slab geometry. In the first he found corrections to the classical critical FKP, following an expansion in powers of a small activation-energy parameter. The remaining two problems involved non-uniform boundary conditions, and were motivated by the very practical problems posed by the use of still thermally active refuse tips for building purposes. In each case a critical temperature distribution and critical FKP has been obtained. With reactant consumption included, these thermal-ignition problems can no longer be treated via a steady-state theory. Boddington, Gray & Kay† considered a class of problems in which not only is reactant consumption included, but also a time-varying ambient temperature. Such problems, whose asymptotic parameter perturbation analysis is based not upon activation energy but upon a dimensionless adiabatic temperature rise, model important experimental situations as, for example, in differential thermal analysis or differential scanning calorimetry. It was demonstrated that increasing the ambient temperature acts in opposition to the reactant consumption rate. Three different rates of heating can be identified which lead to behaviour similar to a decreasing reaction order with increasing rate of heating; ultimately explosion is inevitable and critical states vanish.

Champion†, Deshaies, Joulin & Kinoshita considered the initiation of a lean spherical flame of heavy gaseous fuel. Using high-activation-energy asymptotics they demonstrated the existence of a critical flame radius below which the flame would collapse, and above which it would expand indefinitely. This analytical investigation was supported by numerical work that also agreed well with experimental data obtained with flames in lean propane–air mixtures.

In a pair of related papers Dold, and Kassoy,† Berbernes & Clarke returned to the problem of the 'hot-spot' development in spatially varying thermal runaway using high-activation-energy asymptotics. Dold's contribution was based upon his earlier work (Dold 1979, 1985) which suggests that three matching layers are required to describe the event. Kassoy *et al.*, whilst agreeing that the earlier two-layer models of Kassoy & Poland (1980) and Kapila (1980) are incomplete, suggest that four matching layers are required. It appears that the innermost of these layers, whilst not essential (at least at leading order), motivates the form of variable groupings required in the next layer in a useful way, and augments the largely physical arguments used previously. One might hope that the way is now clear for detailed analysis of gas-phase ignition with coupled generation of pressure waves.

† Denotes the presenter of a multi-author paper.

3. Two-phase problems

Ignition events are also important in pulverised-solid-fuel burners controlled by aerodynamics of the burner jet, and volatilization and ignition of a single coal particle was the subject of a paper by Kordylewski†, Rybak & Zembrzuski. The method of activation-energy asymptotics has been used to follow the course of the ignition process of the volatiles emitted during pyrolysis from the coal particle. Comparison with experiment shows good agreement for large coal particles. For small particles there is a discrepancy which is probably due to the fact that it is not then the volatile material that is responsible for ignition. Of course, for the coal-dust suspension in air that fuels coal-fired power-station burners, a study of the ignition of an isolated particle is not an obviously fruitful approach. Cooper† & Nettleton described a mathematical model of the ignition of a plane flame front in a coal-dust suspension in air. It is based on coal-particle heating via a combination of radiative heat transfer from the main flame and exothermic chemical reactions occurring in the gas phase and at the surface of the particles. The incorporation of experimental information into the model suggests that coal particles heat essentially via radiation from the main flame to an ignition temperature before rates of loss of volatiles and exothermic reactions become significant. The consequences for burner-flame stability were discussed.

Joulin also considered flame propagation in a dust-laden cloud, but in this case a cloud of inert particles. Physically realistic assumptions simplify the governing equations that describe the unsteady competition between radiative pre-heating, particle mixture loading and conductive heat losses. The integro-differential equation that determines flame growth is derived by singular perturbation methods. Numerical solutions of this equation show a transition from slow to fast flames that may be progressive, or sudden in cases when a third (unstable) flame speed is predicted.

In another contribution dealing with single particles, Liñan & Higuera† reconsidered the classical fuel-droplet burning problem. Their concern was with the hydrodynamical stability of the system. They showed that the only instabilities that need be analysed are in the liquid phase, and then only during the transient state when the liquid-droplet temperature is non-uniform. They deduce that, for droplets that are large enough to sustain a diffusion flame, viscous stresses tend to be destabilizing whilst surface tension, including Marangoni effects, have a stabilizing influence.

A related pair of papers by Norbury and by Stuart introduced the subject of combustion in a very porous medium. Norbury was concerned primarily with questions of modelling. Laws of conservation of mass and energy are employed, and the system is closed by a Charles' law form of the gas law with gas momentum calculated from a Darcy law. The reaction is assumed to be two-stage. The first stage represents oxygen leaving the gas and diffusing into the solid. The second stage is the combination of carbon from the solid with the oxygen to form carbon dioxide, which leaves ash and produces heat. Each stage is modelled appropriately and the two are combined to give an overall reaction rate. Norbury also presented numerical solutions for travelling waves in this system. Stuart analysed the stability of these travelling waves by seeking normal mode solutions to the linearised evolutionary equations, and by considering possible bifurcations into spatial dependence in the direction perpendicular to that of the wave propagation.

4. Two-fluid models

Both Philips and Taylor, in separate papers, addressed themselves to the problem of damage that may occur following an accidental explosion in a chemical plant, as for example at Flixborough. Philips drew attention to the inadequacy of model-scale experiments to predict the observed over-pressures, and argued that to achieve detonation of an unconfined vapour cloud not only must the fuel be energetic enough but the cloud and ignition zone must be sufficiently large. He supported his arguments by presenting the results of calculations based on a two-fluid model in which burnt and unburnt fuel are separated by a model turbulent flame front. Conservation equations are invoked for both fluids, and the area of the wrinkled flame surface, momentum transfer across it, and heat release at it are described by empirical formulae. By contrast, Taylor suggested that confined situations will result in the greater damage. Using only balances of mass and momentum across the propagating-flame zone a theoretical model of flame propagation along a gas-filled duct, containing obstacles and vented through the roof, has been developed. Laboratory-scale experiments on flame propagation show good agreement with theory. Perhaps two main issues are involved in these two studies. On the one hand, confinement leads to a purely fluid-dynamical effect to accelerate the flame, whilst for unconfined regions gas-dynamical effects are more significant.

Moss was one of the few contributors to deal with turbulent flow in any more than a general empirical fashion in his paper on the effects of the interaction between turbulence and chemistry on the propagation of pre-mixed flames. His two-fluid model is of the type that is becoming popular for modelling the phenomenon of counter-gradient diffusion. Emphasis was placed on the link between laminar and turbulent flames through the need to construct joint probability density functions based on studies of laminar flames in unsteady and flame-straining flow fields.

5. Gasdynamics and combustion

Flame–acoustic coupling is becoming a subject of increasing importance in combustion, particularly in understanding the stability and resonance of flames and their capacity to produce substantial acoustic power outputs from enclosed regions, where pressure waves interacting with flames may be amplified considerably. McIntosh drew attention to the importance of the parameters formed from the ratios of diffusion time or reaction time to the acoustic time, and outlined results obtained when these parameters take limiting values. In particular, he highlighted the importance that flame structure can have when considering non-adiabatic flames where real density changes are taken into account. Ebert & Schöffel† considered the difficult theoretical problem posed by interaction between a plane shock wave and a cylindrical flame. The interaction leads to a curved shock behind which vorticity is created, leading to a deformation of the deflagration zone. The results are broadly in agreement with experiment, and it is suggested that such an interaction can be identified as a mechanism for generating or amplifying flame turbulence.

Toro† & Fitt were concerned with a quite different type of interaction between fluid dynamics and combustion in their studies of the combustion of solid propellants. A characteristic feature of the gas dynamics associated with solid-propellant gasification is the presence of shock waves and other discontinuities within the flow field. For the simplified one-dimensional model considered, an assessment of the performance of different numerical methods was first made; these were then applied to problems in which ignition and flame spreading are important parts of the process.

The remaining two papers in this section, by Deshaies† & Joulin, and by Clarke, Kassoy & Riley†, were concerned with aspects of detonation initiation. Deshaies & Joulin presented a phenomenological model of turbulent wave propagation behind a precursor shock wave. Situations in which either two values of steady turbulent flame propagation are possible, or none at all, were discussed in the context of deflagration-to-detonation transition phenomena. By contrast, Clarke *et al.* were concerned with the direct initiation of detonation waves that arise when a high level of heat flux is applied over a short time at the boundary of a half-space filled with combustible gas. The response of the gas is described by the equations for the flow of a one-dimensional unsteady fully compressible reactive material that is viscous, heat-conducting and diffusive. Numerical solutions show an initial explosion at the boundary that drives a shock into the undisturbed gas. The trailing reaction wave eventually accelerates to overtake the shock and, following a violent transient interaction within which high pressures develop, a steady detonation wave of ZND-type emerges.

6. Chemical kinetics and flames

Contrary to what may be supposed, chemists are no more enamoured of very large reaction schemes than combustion scientists. That large reaction schemes are involved in combustion phenomena cannot be doubted. For the methane flame perhaps a couple of hundred steps are involved, although for lean flames this is readily reduced to 18 steps involving 13 species. Peters & Donnerhack† showed how for these lean flames this scheme may be reduced to four overall reaction steps. They have obtained results from this that compare well both with results from the full scheme for lean flames and with experiment. Liñan considered the ozone flame using a reaction scheme that is both well accepted, and simple enough to handle using asymptotic methods. He first examined the steady structure, and showed how an endothermic reaction step that is included in the reaction scheme has a significant effect on the flame structure. He found a part of this structure that is very similar to a diffusion flame, where radicals have an important role to play, and which makes the flame sensitive to disturbances in the upstream flow.

David†, Bloor, Dixon-Lewis & Gaskell consider the structure of the counterflow diffusion flame close to the forward stagnation region of a porous cylinder from which gaseous fuel is ejected, as in the experiment of Tsuji & Yamaoka (1971). Their technique involves a series expansion close to the stagnation point, and the solutions obtained show the basic variations in flow velocities, pressure, temperature and chemical composition for a flame that is strained by its ambient flow.

In his study of turbulent-jet diffusion flames with complex chemistry, Rogg incorporates the effects of chemical reaction into his turbulence model by introducing an ensemble of microscopic flamelets along the surface of the turbulent flame. Each flamelet represents a counter-flow diffusion flame, with simulated stretch effects, into which as many as 50 reaction steps are incorporated. Numerical results have been obtained for jets of methane in still air, and jets of carbon monoxide in coflowing air. Comparisons with experiment confirm the effectiveness of this approach to the incorporation of complex chemistry into turbulent flow-field predictions.

Clavin†, Fife & Nicolaenko introduce three model, as opposed to real, two-reaction schemes, and the consequences of such a competitive chemical situation are explored. For each scheme the solutions for steady plane premixed flames present either an S-shaped curve or a plateau, when the adiabatic flame temperature is plotted against the reduced mass fraction of the limiting reactant, depending upon the relative magnitudes of the two chemical heat releases. For the S-shaped curve a stability analysis has been carried out in the vicinity of the turning points (corresponding to extinction and ignition) which are therefore proved to delimit the stable and unstable branches of the curve.

REFERENCES

(An asterisk indicates a lecture given at the Colloquium.)

ADLER, J.* Criticality criteria for thermal explosions.

BODDINGTON, T., GRAY, P. & KAY, S.* Times to ignition in exothermic systems in steadily heated surroundings.

CHAMPION, M., DESHAIES, B., JOULIN, G. & KINOSHITA, K.* Initiation of lean flames of heavy gaseous fuel; seeking for limiting mechanisms.

CLARKE, J. F., KASSOY, D. R. & RILEY, N.* Detonation wave initiation by rapid energy deposition at a confining boundary.

CLAVIN, P., FIFE, P. & NICOLAENKO, B.* Competing-reaction flames.

COOPER, S. & NETTLETON, M. A.* The ignition of pulverised coal flames.

DAVID, T., BLOOR, M. I. G., DIXON-LEWIS, G. & GASKELL, P. H.* Direct coordinate expansions for counterflow diffusion flames.

DESHAIES, B. & JOULIN, G.* A tentative sufficient criterion for deflagration to detonation transition.

DOLD, J. W.* The role of thermal runaway in the ignition process.

DOLD, J. W. 1979 Ph.D. thesis, Cranfield Institute of Technology.

DOLD, J. W. 1985 *Q. J Mech. Appl. Maths* **38**, 361.

EBERT, F. & SCHÖFFEL, S. U.* Calculation of the flow-field caused by shock wave and deflagration interaction.

JOULIN, G.* Radiation-affected dynamics of spherical flames in particle-laden gaseous mixtures.

KAPILA, A. K. 1980 *SIAM J. Appl. Maths* **39**, 21.

KASSOY, D. R. & POLAND, J. 1980 *SIAM J. Appl. Maths* **39**, 412.

KASSOY, D. R., BEBERNES, J. & CLARKE, J. F.* The thermal-explosion solution.

KORDYLEWSKI, W., RYBAK, W. & ZEMBRZUSKI, M.* Dynamics of coal particle ignition.

LIÑAN, A. & HIGUERA, F. J.* Droplet vaporization in a stagnant hot atmosphere without free or forced convection.

LIÑAN, A.* The ozone flame.

MCINTOSH, A. C.* Flame–acoustic coupling.

MOSS, J. B.* Turbulence–chemistry interaction effects on pre-mixed flame propagation.

NORBURY, J.* Modelling combustion in a porous medium.

PETERS, N. & DONNERHACK, S.* Numerical analysis of a systematically reduced reaction scheme for methane flames.

PHILIPS, H.* Flame acceleration in vapour-cloud explosions.

ROGG, B.* Application of the laminar flamelet model to turbulent jet diffusion flames with complex chemistry.

STUART, A.* Travelling combustion waves in a porous medium.

TAYLOR, P. H.* On the role of fast-flame propagation in congested regions.

TORO, E. F. & FITT, A. D.* Theoretical and numerical aspects of the gas dynamics associated with the combustion of a solid propellant.

TSUJI, H. & YAMAOKA, I. 1971 *Thirteenth Symp. (International) on Combustion* (Combustion Institute, Pittsburgh), p. 723.

WILLIAMS, F. A. *Combustion Theory*, 1st edn, 1965, Academic: 2nd edn, 1985, Benjamin/Cummings.